# MICHTOX: A Mass Balance and Bioaccumulation Model for Toxic Chemicals in Lake Michigan

## Ronald Rossmann, Editor

Large Lakes and Rivers Forecasting Research Branch
Mid-Continent Ecology Division
National Health and Environmental Effects Research Laboratory
Office of Research and Development
Large Lakes Research Station
9311 Groh Road
Grosse Ile, Michigan 48138

September 2005



## **Notice**

The information in this document has been obtained primarily through funding by the United States Environmental Protection Agency (USEPA) under the auspices of the Great Lakes National Program Office (GLNPO) and the Office of Research and Development (ORD). The report has been subjected to the Agency's peer and administrative review and it has been approved for publication as a USEPA document. Mention of trade names or commercial products does not constitute endorsement or recommendation for use. Because the purpose of this report is to document the development of the MICHTOX model, conclusions are historical and should not be considered current.

## **Foreword**

Federal and contractor staff at the United States Environmental Protection Agency's Large Lakes Research Station have been involved with the development of mass balance models for the Great Lakes since the early 1970s. MICHTOX is a mass balance model developed to predict chemical concentrations in water and sediments of Lake Michigan in response to chemical loads to the lake. The model was adapted from the general water quality model WASP4. The MICHTOX bioaccumulation model was based upon the WASTOXv4 food chain model. Development of MICHTOX began in the early 1990s. The model was developed as a planning tool for the Lake Michigan Mass Balance Project (LMMBP) (U.S. Environmental Protection Agency, 1997). This work was documented in an in-house report in 1992 (Part 1). The model was applied as a screening-level model for atrazine in Lake Michigan in support of the LMMBP (Rygwelski et al., 1999). The model was slightly revised and applied to polychlorinated biphenyls (PCBs) in Lake Michigan to confirm model results with the LMMBP project data and to provide preliminary modeling results for inclusion in the 2002 Lakewide Management Plan (LaMP) report (Lake Michigan Technical Committee, 2002). These were reported in a 2002 contractor report (Part 2). The purpose of this report is to document through 2002 the progression of MICHTOX model development and application of the model to describing the behavior of contaminants. especially PCBs, in Lake Michigan. Both parts of this report have been cited numerous times in the literature. This report provides ready access to these for interested parties. For PCBs, results from application of the model have been superceded by more recent results.

Lake Michigan Technical Committee. 2002. Lake Michigan Lakewide Management Plan (LaMP), 2002. U.S. Environmental Protection Agency, Great Lakes National Program Office, Chicago, Illinois. 102 pp.

Rygwelski, K.R., W.L. Richardson, and D.D. Endicott. 1999. A Screening-Level Model Evaluation of Atrazine in the Lake Michigan Basin. J. Great Lakes Res., 25(1):94-106.

U.S. Environmental Protection Agency. 1997. Lake Michigan Mass Budget/Mass Balance Work Plan. U.S. Environmental Protection Agency, Great Lakes National Program Office, Chicago, Illinois. EPA/905/R-97/018, 155 pp.

## **Abstract**

MICHTOX is a toxic chemical mass balance and bioaccumulation model for Lake Michigan. It was developed for the United States Environmental Protection Agency's Region V in support of the Lake Michigan Lake-wide Management Plan (LaMP) to provide guidance on expected water guality improvements in response to critical pollutant loading reductions. The 11 critical pollutants modeled were benzo(a)pyrene, chlordane, total dichlorodiphenyltrichloroethane (DDT), dieldrin, heptachlor epoxide, hexachlorobenzene, lead, total polychlorinated biphenyls (PCBs), 2,3,7,8-tetrachlorodibenzo-p-dioxin (TCDD), 2,3,7,8-tetrachlorodibenzofuran (TCDF), and toxaphene. Concentrations of these were predicted in 17 water and sediment segments in response to atmospheric and tributary loadings. The bioaccumulation model was coupled to the mass balance model to predict chemical accumulation in lake trout and bloater through pelagic and benthic food chains. Mass balance predictions were validated using plutonium, lead, and PCBs data; and bioaccumulation predictions were validated with PCBs data. The model was later applied to provide preliminary PCBs model results for the Lake Michigan Mass Balance Project. Results from this application were used to guide the development of a more resolute model for PCBs. Results for PCBs described in Part 1 are superceded by results in Part 2. Part 2 results have been replaced by a more recent application of MICHTOX that has been presented at various meetings and will be published at a future date. This document is meant to provide a historical perspective of MICHTOX development and application.

# **Table of Contents**

			iv
			viii
			Xiv
			XV
	_		xvii
Execu	tive Sur	mmary	xviii
Part 1	1992 N	иіснтох:	A Mass Balance and Bioaccumulation Model for Toxic
	Chem	icals in Lak	e Michigan
	1.1	Evocutivo	Summary
	1.1		Summary
	1.2	1.2.1	Verification of Model Predictions
		1.2.1	
			1.2.1.1 Air Concentrations/Deposition Fluxes31.2.1.2 Surficial Sediment Concentrations3
			1.2.1.2 Sumicial Segiment Concentrations
			1.2.1.3 Lake Trout
			1.2.1.4 Major Tributaries
		4.0.0	1.2.1.5 Water
		1.2.2	Extend Model to Other Critical Pollutants and Target Organisms
		1.2.3	Further Model Development
			1.2.3.1 Circulation
			1.2.3.2 Sediment Transport
			1.2.3.3 Organic Carbon Dynamics
			1.2.3.4 Food Chain Variability and Dynamics
		1.2.4	Establish Linkages to Atmospheric and Watershed Models
	1.3		on
		1.3.1	Project Objectives
		1.3.2	Lake Michigan Toxics Problem
	1.4		scription
		1.4.1	Model Framework
		1.4.2	Segmentation
		1.4.3	Circulation 12
		1 1 1	Solids Balance 13

	1.4.5	Chemical Partitioning and Loss
		1.4.5.1 Partitioning
		1.4.5.2 Volatilization
		1.4.5.3 Photolysis
		1.4.5.4 Sediment-Water Diffusive Exchange
	1.4.6	Chemical Loads and Boundary Conditions
		1.4.6.1 Atmospheric Deposition
		1.4.6.2 Tributary Loads
		1.4.6.3 Loading Histories
		1.4.6.3.1 Plutonium
		1.4.6.3.2 Lead
		1.4.6.3.3 PCBs
		1.4.6.4 Lake Huron Boundary Conditions
	1.4.7	Chemical Bioaccumulation
	1. 1.7	1.4.7.1 Food Chain
		1.4.7.2 Uptake Rate
		1.4.7.3 Elimination Rate
		1.4.7.4 Dietary Accumulation
		1.4.7.5 Modeling the Base of the Food Chain
	1.4.8	Steady-State Model
	1.4.9	Chemical-Specific Parameterization
1.5	Model Val	· ·
1.5	1.5.1	Plutonium
	1.5.1	Lead
	1.5.2	PCBs
	1.5.5	1.5.3.1 Water
		1.5.3.2 Sediment
		1.5.3.3 Biota
		1.5.3.4 Bioaccumulation
1.6	Staady-St	ate Model Applications
1.0	1.6.1	Steady-State Load-Response Predictions
	1.6.2	Mass Fate and Transport
	1.6.3	Sensitivity Analysis
	1.6.4	Uncertainty Analysis
	1.0.4	1.6.4.1 Analysis of Model Uncertainty
		1.6.4.2 Results
		1.6.4.3 Critical Parameterization Uncertainty
1.7	Dynamic I	Model Applications
1.1	1.7.1	Toxic Chemical Lag Time
	1.7.1	PCBs Fate and Transport Fluxes in Dynamic Simulations
	1.7.3	Additional Dynamic Simulations for PCBs
	1.7.3	1.7.3.1 PCBs Control Scenarios
		1.7.3.1 FCBs Control Scenarios
	1.7.4	Uncertainty in Dynamic Simulations
1.8	Reference	
1.9		Steady-State Model Output for Each Toxic Chemical
1. <i>U</i>	TADDCHUIA.	Dicady Diato Model Daibai for Each 19010 Offellical

Part 2			an Mass Balance Project: Modeling Total Polychlorinated Biphenyls OX Model	84
	2.1		Summary	84
	2.2	Recomme	ndations	85
	2.3	Introduction	on	85
	2.4	Description	n of Model, Data, and Simulations	86
		2.4.1	MICHTOX Model	86
		2.4.2	Mass Balance Data for PCBs	90
		2.4.3	Revised MICHTOX and LMMBP Forcing Functions	94
	2.5	Results ar	nd Discussion	98
		2.5.1	Confirmation of MICHTOX PCBs Bioaccumulation Predictions	98
		2.5.2	Comparison of Original MICHTOX PCBs Simulations to the	
				104
		2.5.3	-1	109
		2.5.4	1 5	110
		2.5.5	3	110
		2.5.6		129
		2.5.7	•	131
		2.5.8	Are Lake Michigan Total PCBs Concentrations in Equilibrium With	
			I I	131
		2.5.9	Sensitivity of Bioaccumulation Predictions to Initial Total PCBs	
				132
		2.5.10	Sensitivity of Bioaccumulation Predictions to Food Chain Model	
				132
		2.5.11	Are Total PCBs Bioaccumulation Factors Constant for Lake Trout	
				136
	2.6	Reference	9S	136

# **List of Figures**

1.1	Long-term concentration trends for toxic chemicals in small Lake Michigan fish	7
1.2	MICHTOX mass balance schematic	9
1.3	Spatial segmentation for the 17 segment MICHTOX model	11
1.4	Results of chloride calibration of Green Bay dispersive exchange	13
1.5	Suspended particle calibration	14
1.6	Organic carbon fraction of surface water particles	15
1.7	Partitioning model: Sensitivity of dissolved chemical fraction to non-settling organic matter binding efficiency	16
1.8	Calibration of partitioning model: Comparison to distribution coefficient data for HOCs in the Great Lakes	17
1.9	Sensitivity of computed volatilization rate to wind speed and temperature (pentachlorobiphenyl)	18
1.10	Plutonium deposition to Lake Michigan	20
1.11	Total loading of lead to Lake Michigan	20
1.12	PCBs loading time function and comparison to reported PCBs load estimates	22
1.13	MICHTOX food chain structure	24
1.14	Chemical assimilation efficiency for <i>Mysis</i> calculated from Lake Ontario PCBs data	26
1.15	Chemical assimilation efficiency for alewife calculated from Lake Ontario HOCs data	26
1.16	Chemical assimilation efficiency for <i>Diporeia</i> calculated from Lake Ontario PCBs data	26
1.17	Steady-state spreadsheet model for pentachlorobiphenyl (PCB5)	27
1.18	Simplified Lake Michigan lake trout food chain	28

1.19	overturn data)	31
1.20	MICHTOX simulation of plutonium in southern Lake Michigan (epilimnion, hypolimnion, and seasonal epilimnetic data)	31
1.21	MICHTOX simulation of plutonium in southern Lake Michigan – sensitivity to vertical segmentation	32
1.22	Simulation of annual-averaged lead concentrations in southern Lake Michigan	32
1.23	Lead simulation in southern Lake Michigan surficial sediment	32
1.24	Simulation of PCBs in southern Lake Michigan	33
1.25	Simulation of PCBs in Green Bay	33
1.26	PCBs simulations in central Lake Michigan and outer Green Bay	34
1.27	PCBs simulations in Lake Michigan and outer Green Bay surficial sediments	34
1.28	PCBs simulations in Green Bay sediments	34
1.29	Simulated PCBs distribution in southern Lake Michigan sediments	35
1.30	PCBs concentrations in Lake Michigan lake trout	35
1.31	Verification of PCBs accumulation in age seven lake trout	36
1.32	Sensitivity of trout PCBs predictions to the food chain	36
1.33	Verification of PCBs accumulation predictions in lake trout age classes 2-9	37
1.34	Simulation of PCBs concentrations in age 2-12 trout, 1980-1989	37
1.35	Simulation of PCBs concentrations in age 2-12 trout, 1980-1990	37
1.36	Verification of PCBs concentration predictions for bloater	38
1.37	Validation of bioaccumulation predictions for lower trophic levels in Lake Michigan	39
1.38	MICHTOX predicted trout bioaccumulation and data from Lake Ontario	40
1.39	MICHTOX predicted trout biota-to-sediment ratio and data from Lake Ontario	41
1.40	Load-concentration relationship for PCBs in southern Lake Michigan	42
1.41	Relative magnitude of PCBs fate and transport fluxes	43
1.42	PCBs air-water fluxes at steady-state in southern Lake Michigan	44

1.43	Sensitivity of water concentrations to K <sub>ow</sub>	44
1.44	Sensitivity of trout concentrations to K <sub>ow</sub>	44
1.45	Sensitivity to Henry's constant	45
1.46	Sensitivity to volatilization rate	45
1.47	Sensitivity to dry deposition velocity	45
1.48	Sensitivity to sediment-water diffusion coefficient	45
1.49	Sensitivity of trout concentration to chemical assimilation efficiency	46
1.50	Sensitivity of trout concentration to pelagic diet fraction of forage fish	46
1.51	Sensitivity to dispersive exchange coefficient	46
1.52	Sensitivity to suspended particle concentration	46
1.53	Sensitivity to particle burial velocity	47
1.54	Sensitivity to particle settling velocity	47
1.55	Sensitivity of water concentrations to suspended particle $f_{oc},\ldots,$	47
1.56	Sensitivity of sediment concentrations to suspended particle $f_{oc} \dots \dots \dots$	47
1.57	Sensitivity of trout concentrations to suspended particle $f_{oc}$	48
1.58	MICHTOX steady-state response to different tributary load distributions	48
1.59	Load-concentration relationship for PCBs in southern Lake Michigan including confidence limits	53
1.60	Load-concentration relationship for PCBs in southern Lake Michigan water:  Effect of constant air concentration	55
1.61	Load-concentration relationship for PCBs in southern Lake Michigan trout:  Effect of constant air concentration	55
1.62	Contribution of critical parameters to steady-state model uncertainty: Water concentration	55
1.63	Contribution of critical parameters to steady-state model uncertainty: Trout concentration	56
1.64	Predicted PCBs time response to loading reduction in southern Lake Michigan	58
1.65	Response of trout PCBs concentrations at various times after reducing PCBs load	58

1.66	Resources, 1990)	59
1.67	Simulation of DDT in Lake Michigan trout (DeVault <i>et al.</i> , 1986; Michigan Department of Natural Resources, 1990)	59
1.68	Simulation of dieldrin in Lake Michigan trout (DeVault <i>et al.</i> , 1986; Michigan Department of Natural Resources, 1990)	59
1.69	Load cutoff simulation of PCBs in Lake Michigan trout	59
1.70	Tetrachlorodibenzo-p-dioxin simulation in Lake Michigan trout (U.S. Environmental Protection Agency, 1989b)	60
1.71	Tetrachlorodibenzofuran simulation in Lake Michigan trout (U.S. Environmental Protection Agency, 1989b)	60
1.72	Predicted effectiveness of PCBs load reductions	61
1.73	Simulation of storm event in southern Lake Michigan	62
1.74	Effect of storm event on PCBs in southern Lake Michigan sediment	62
1.75	Sensitivity of PCBs concentrations in trout to thin (1.1 cm) surficial sediment layer thickness	63
1.76	Predicted water PCBs concentrations for ten realizations of dynamic model	63
1.77	Predicted trout PCBs concentrations for ten realizations of dynamic model	64
2.1	MICHTOX mass balance schematic	87
2.2	Spatial segmentation for the 17 segment MICHTOX model	88
2.3	The LMMBP estimates of total PCBs atmospheric vapor concentrations processed as monthly values for MICHTOX Segments 1-3	91
2.4	The LMMBP estimates of total PCBs atmospheric wet and dry deposition processed as monthly values for MICHTOX Segment 1 (southern Lake Michigan)	92
2.5	The LMMBP estimates of total PCBs tributary loading processed as monthly values for MICHTOX Segment 1 (southern Lake Michigan)	93
2.6	Long-term estimates of Lake Michigan total PCBs vapor concentrations	99
2.7	Long-term estimates of Lake Michigan total PCBs atmospheric deposition loading	100
2.8	Long-term estimates of Lake Michigan total PCBs tributary loading	101

2.9	data steady-state total PCBs concentrations to Saugatuck fish	102
2.10	Comparison of MICHTOX steady-state total PCBs concentrations to Sheboygan Reef fish data	103
2.11	Original MICHTOX predictions and data for main lake total PCBs concentrations	105
2.12	Original MICHTOX predictions and data for main lake sediment total PCBs concentrations (sediment cores collected in 1991-1992)	106
2.13	Original MICHTOX predictions of total PCBs concentrations in fish and comparison to Sheboygan Reef zone data	107
2.14	Original MICHTOX predictions of total PCBs concentrations in lake trout and comparison to DeVault <i>et al.</i> (1986) data	108
2.15	Long-term Scenario A predictions of main lake total PCBs concentrations	111
2.16	MICHTOX southern Lake Michigan total PCBs predictions. Comparison of long-term Scenario A to original model predictions	112
2.17	Comparison of long-term Scenario A predictions to main lake sediment total PCBs concentrations (sediment cores collected in 1991-1992)	113
2.18	Comparison of long-term Scenario A predictions to DeVault et al. (1986) lake trout data	114
2.19	Comparison of MICHTOX Scenario A total PCBs concentrations to Sheboygan Reef data	115
2.20	Long-term Scenario B predictions of main lake total PCBs concentrations	117
2.21	MICHTOX southern Lake Michigan total PCBs predictions. Comparison of long-term Scenario B to original model predictions	118
2.22	Comparison of long-term Scenario B predictions to the LMMBP deepwater dissolved total PCBs concentrations	119
2.23	Comparison of Scenario B predictions to main lake sediment total PCBs concentrations (sediment cores collected in 1991-1992)	120
2.24	Comparison of long-term Scenario B predictions to average total PCBs sediment concentrations (LMMBP and GBMBP box core samples)	121
2.25	Comparison of long-term Scenario B predictions to DeVault et al. (1986) lake trout data	122
2.26	Comparison of long-term Scenario B total PCBs concentrations to Sheboygan Reef fish data	123
2.27	Long-term Scenario C predictions of main lake total PCBs concentrations	124

2.28	MICHTOX southern Lake Michigan total PCBs predictions. Comparison of long-term Scenario C to original model predictions	125
2.29	Comparison of Scenario C predictions to main lake sediment total PCBs concentrations (sediment cores collected in 1991-1992)	126
2.30	Comparison of long-term Scenario C predictions to DeVault <i>et al.</i> (1986) lake trout data	127
2.31	Comparison of MICHTOX Scenario C total PCBs concentrations to Sheboygan Reef fish data	128
2.32	Toxic chemical management alternatives. Comparison of forecast simulation for age seven lake trout in southern Lake Michigan	130
2.33	Total PCBs concentrations in Lake Michigan air and water	133
2.34	Ratio of total PCBs concentrations between dissolved water and vapor (MICHTOX No-Action forecast)	134
2.35	Sensitivity of food chain model to initial conditions. Age seven lake trout: No-Change forecast	135
2.36	Sensitivity of MICHTOX steady-state PCBs concentrations to chemical assimilation efficiency and comparison to Saugatuck biota zone data	137
2.37	Predicted bioaccumulation factors for total PCBs in age seven lake trout (No-Change forecast simulation)	138

# **List of Tables**

1.1	Sediment Segment Parameterization	13
1.2	Particle Flux Parameterization	14
1.3	Selected Air Concentrations and Calculated Atmospheric Deposition Loadings for Lake Michigan Priority Pollutants	19
1.4	Octanol-Water Partition Coefficient $(K_{ow})$ and Organic Carbon Partition Coefficient $(K_{oc})$ for Lake Michigan Priority Toxics	29
1.5	Physicochemical Parameters Used in Volatilization Parameterization of Lake Michigan Critical Pollutants	29
1.6	Volatilization Rate Parameters for Lake Michigan Critical Pollutants	30
1.7	Photolysis Rate for Lake Michigan Critical Pollutants	30
1.8	Predicted Steady-State Bioaccumulation Factors (BAFs) for Critical Pollutants in Lake Michigan Lake Trout	40
1.9	Predicted Steady-State Concentrations of Critical Pollutants in Lake Michigan for Unit Loading	42
1.10	Summary of Mass Fate and Transport for Critical Pollutants in Lake Michigan.  Southern Lake Michigan Mass Fluxes Expressed as Fractions of Segment Load	43
1.11	Comparison of PCBs Mass Fate and Transport for Critical Pollutants in Southern Lake Michigan and Central Green Bay	43
1.12	Probability Distribution for Steady-State Model Uncertainty Analysis	51
1.13	Summary of Results for First Test of Model Uncertainty. Predicted Steady-State Concentrations for Fixed Air Concentrations of 1 ng/m³ for Each Chemical	52
1.14	Summary of Results for Second Test of Model Uncertainty. Predicted Steady-State Concentrations for Expected Air Concentrations of Each Chemical	53

1.15	Summary of Results for Third Test of Model Uncertainty. Predicted Steady-State PCBs Concentrations for Varying Tributary Loads and Expected Air Concentrations	54
1.16	Predicted Long-Term Chemical Loss Rates for Lake Michigan Critical Pollutants Following Loading Reduction. First-Order Loss Rates in Units of 1/Year in Southern Lake Michigan	57
2.1	Cruise- and Segment-Specific Dissolved Fraction of Total PCBs Concentrations (ng/L)	94
2.2	Cruise- and Segment-Specific Average Particulate Total PCBs Concentrations (ng/L)	94
2.3	Segment-Specific Average Surficial Sediment Total PCBs Concentrations (ng/g)	95
2.4a	Average Total PCBs Concentrations in Fish in the Saugatuck Biota Zone	95
2.4b	Average Total PCBs Concentrations in Fish in the Sheboygan Reef Biota Zone	96
2.4c	Average Total PCBs Concentrations in Fish in the Sturgeon Bay Biota Zone	96
2.5	Comparison of Original MICHTOX Total PCBs Forcing Functions for 1994-1995 to the LMMBP Estimates (Whole-Lake Average)	104
2.6	Mass Balance Diagnostics for Total PCBs in the Original MICHTOX Simulation (Year 1994-1995)	109
2.7	Comparison of Original and Revised Henry's Constant (atm m³/mol) Parameterization	110
2.8	Monthly PCBs Volatilization Rates (m/d) Calculated by Original and Revised MICHTOX Formulations	111
2.9	Mass Balance Diagnostics for Total PCBs in MICHTOX Scenario B Simulation (Year 1994-1995)	127
2.10	MICHTOX Predictions of Total PCBs Concentrations (µg/g) in Lake Trout for Toxic Chemical Management Alternatives	131
2.11	Results of BMC Uncertainty Analysis for Original Steady-State MICHTOX Model	132

#### **Abbreviations**

AOCs Areas of Concern
BAF Bioaccumulation factor

BaP Benzo(a)pyrene

BCF Bioconcentration factor
BMC Bayesian Monte Carlo
BSF Biota-to-sediment factor
BSR Biota-to-sediment ratio
CV Coefficient of variance

DDD Dichlorodiphenyldichloroethane Dichlorodiphenyldichloroethylene DDE DDT Dichlorodiphenyltrichloroethane **EPRI** Electric Power Research Institute ERL Environmental Research Laboratory **GBMBP** Green Bay Mass Balance Project Great Lakes Environmental Center GLEC Great Lakes National Program Office GLNPO

HCB Hexachlorobenzene

HOCs Hydrophobic organic chemicals LaMP Lake-wide Management Plan

LCL Lower confidence limit

LMMBP Lake Michigan Mass Balance Project

LLRFRB Large Lakes and Rivers Forecasting Research Branch

LLRS Large Lakes Research Station
InCV Lognormal coefficient of variance

MDNR Michigan Department of Natural Resources

MED Mid-Continent Ecology Division
NSOM Non-settling organic matter
PCBs Polychlorinated biphenyls
PCB4 Tetrachlorobiphenyl
PCB5 Pentachlorobiphenyl

PCDD Pentachlorodibenzo-p-dioxin
PCDF Pentachlorodibenzofuran
QAPP Quality Assurance Project Plan
TCDD Tetrachlorodibenzo-p-dioxin
TCDF Tetrachlorodibenzofuran
UCL Upper confidence limit

USEPA United States Environmental Protection Agency

USFWS United States Fish and Wildlife Service

VWA Volume-weighted average

## **Acknowledgments**

Special thanks for the assistance and cooperation of the federal and on-site contractor staff at the U.S. Environmental Protection Agency, Office of Research and Development, National Health and Environmental Effects Research Laboratory, Mid-Continent Ecology Division-Duluth, Large Lakes Research Station, Grosse Ile, Michigan. David Griesmer, Xiangsheng Xia, Katie Taunt, Xiaomi Zhang, and Xin Zhang provided raw and processed Lake Michigan Mass Balance Project and historical data used for the modeling. Wilson Melendez provided programming support for the necessary modifications of MICHTOX mass balance, food web bioaccumulation, and post-processing programs. Thanks to Kay Morrison for the graphic renditions and figures and to Debra Caudill for formatting and word processing.

## **Executive Summary**

MICHTOX is a toxic chemical mass balance and food chain bioaccumulation model that was first developed in the early 1990s. A Bayesian Monte Carlo uncertainty analysis demonstrated that MICHTOX predicted polychlorinated biphenyl (PCBs) concentrations should be within a factor of two of the measured data. During the early part of the Lake Michigan Mass Balance Project (LMMBP), MICHTOX was updated and used as a preliminary assessment tool of the LMMBP PCBs data and to provide a screening-level analysis of the potential future trends in total PCBs concentrations in Lake Michigan water, sediment, and fish under a variety of contaminant load scenarios.

As reported in 1992, the model predicted the response of Lake Michigan, and with additional resolution, Green Bay to atmospheric and tributary loadings. With its bioaccumulation component, chemical accumulation in biota was predicted in response to the loadings. The model is capable of either dynamic or steady-state simulations. Dynamic model predictions were used to predict the long-term rate of concentration decline following load reduction for each toxic chemical. Significant reductions of PCBs in lake trout were predicted for 2000 with no additional loading reductions. Additional reductions of PCBs concentrations could only be achieved with significant reductions in atmospheric sources. These results were uncertain because PCBs loading history is poorly defined and because of potential error in the parameterization of the surficial sediment layer thickness. The thickness of this layer was demonstrated to be a critical factor in model uncertainty. Additional factors leading to model uncertainty included uncertainty in initial concentrations and loading history and dynamics of the Lake Michigan trophic structure.

As reported in 2002, MICHTOX was used to provide a preliminary mass balance modeling assessment of PCBs in Lake Michigan. Because PCBs vapor concentrations from the LMMBP were significantly higher than estimated in the original model, total PCBs forcing functions were recalculated using the LMMBP estimates. Recommended changes to the model increased the volatilization mass transport rates, resulting in the PCBs equilibrium shifting significantly towards the atmospheric vapor phase quicker than previously predicted. This demonstrated that air-water fluxes predominated the transport pathways for PCBs in Lake Michigan. The best prediction of PCBs concentrations in water, sediment, and fish were obtained with the forcing function peaking in 1961-1963. This was different than the original model simulation reported in 1992. The model was used to forecast total PCBs concentrations in lake trout for a variety of scenarios representing alternative strategies for managing PCBs in Lake Michigan. Because of model uncertainty, observed average total PCBs concentrations should be within a factor of two of predicted values. The bioaccumulation predictions were not sensitive to initial conditions but were sensitive to model parameterization. The PCB predictions of this model are historic and have been replaced by the predictions derived from the improved models used for the LMMBP.